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Electron in quasiplane superlattice of cylindric quantum dots

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Abstract. The theory of electron spectrum in quasiplane superlattice of cylindric quantum dots is built using the modified method of augmented plane waves. It is established that quasiplane energy bands arise only when the ratio between cylinder height and radius of base is bigger than some critical value.

Experimental investigation of periodical semiconductor quantum dots structures started recently [1]. The theory of quasiparticle spectra in such systems and in quantum well superlattices is not established yet.

The theory of electron spectrum in quasiplane quantum superlattice of cylindric quantum dots (Fig. 1) is built. It is assumed that cylindric quantum wells superlattice (CQWS) is embedded into vacuum. The quantum well is a cylinder of height h and radius a; c-distance between the nearest borders of two neighbour dots. Effective mass of electron in the well is μ_1 and in the matrix-μ_2. Well and matrix potentials respectively the vacuum are $(-V_1)$ and $(-V_2)$ consequently. The CQWS system is assumed as infinitly deep potential well because the vacuum surrounding CQWS is a strong potential barrier.

In order to obtain the electron spectrum one has to solve the stationary Schrödinger equation with Hamoltonian

$$\hat{H} = -\frac{\hbar^2}{2}\left(\vec{\nabla}_{xy\varphi}\frac{1}{\mu(x,y)}\vec{\nabla}_{xy\varphi} + \frac{1}{\mu(x,y)}\frac{\partial^2}{\partial z^2}\right) + U(x,y,z). \tag{1}$$

In Cartezian coordinate system where OZ axis is directed along the axial axis of cylinder and OXY plane crossing the middle of cylinders height the potential $U(x,y,z)$ can be written in the form

$$U(x,y,z) = U(x,y) + \begin{cases} 0 & z < h/2 \\ \infty & z \geq h/2 \end{cases} \tag{2}$$

$$U(x,y) = \begin{cases} -V_1 & x, y \ \textit{inside the wells} \\ -V_2 & x, y \ \textit{outside the wells} \end{cases} \tag{3}$$

Introducing the electron average effective mass $\overline{\mu} = (\mu_1+\mu_2)/2$ the electron wave function is found as

$$\psi(x,y,z) = \psi_{||}(x,y)f(z) \tag{4}$$

where

$$f(z) = \begin{cases} \sqrt{\frac{2}{h}}\cos\frac{\pi n}{h}z & n = 1,3,5,... \\ \sqrt{\frac{2}{h}}\sin\frac{\pi n}{h}z & n = 2,4,6,... \end{cases} \tag{5}$$

Thus equation (1) can be rewritten in the form

$$\left\{-\frac{\hbar^2}{2}\left(\vec{\nabla}_{xy}\frac{1}{\mu(x,y)}\vec{\nabla}_{xy}\right) + U(x,y) - E_\perp^0\right\}\psi_\perp^0 = 0 \tag{6}$$

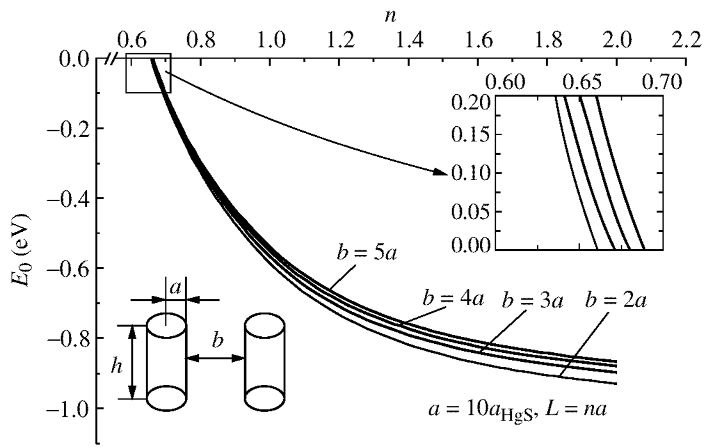

Fig. 1. Electron qround zone dependence on distance between nearest wells, $L = 2\rho_0$.

where

$$E_{\perp}^{0} = E^{0} - \frac{\pi^2\hbar^2}{2\bar{\mu}h^2}n^2. \tag{7}$$

Further equation (6) is solved using the modified method of augmented plane waves (established recently in [2]) for the plane superlattice of circle quantum wells. According to this method one has to write the Schrödinger equation for the wave function inside the plain circle quantum well. In polar coordinate system for the radial function $f_m(\rho)$ it is written as

$$\left\{-\frac{\hbar^2}{2\mu_1}\left[\frac{1}{\rho}\frac{d}{d\rho}\left(\rho\frac{d}{d\rho}\right) - \frac{m^2}{\rho^2}\right] - U_0 + \frac{\pi^2\hbar^2}{2\bar{\mu}h^2}n^2 - E^0\right\} f_m(\rho) = 0 \tag{8}$$

where $U_0 = U_1 - U_2$.

When the energy $\varepsilon = -E < 0$ the solution of equation (8) is Bessel function

$$f_m(\rho) = J_m(\alpha\rho) \tag{9}$$

where

$$\alpha = \sqrt{2\mu_1\hbar^{-2}a^{-2}(U_0 - \epsilon) - \frac{\mu_1}{\bar{\mu}}\frac{n^2}{h^2}}. \tag{10}$$

One can obtain the electron spectrum in quasiplane superlattice of cylindric quantum dots using the function (9) together with the plane waves in modified method of augmented plane waves.

The calculations was performed for the system of β-HgS dots embedded into β-CdS matrix. The results are shown in Figs. 1 and 2. The main conclusions are following.

It is clear from Fig. 1 that plane enrgy bands of superlattice arise only at some critical minimal ratio between cylinder height (h) and radius of base (a); the distance (b) between the neighbour dots is arbitrary. It is clear from physical considerations because at small sizes of any quantum well it cannot produce the bound state creating the band due to the interaction with the other wells.

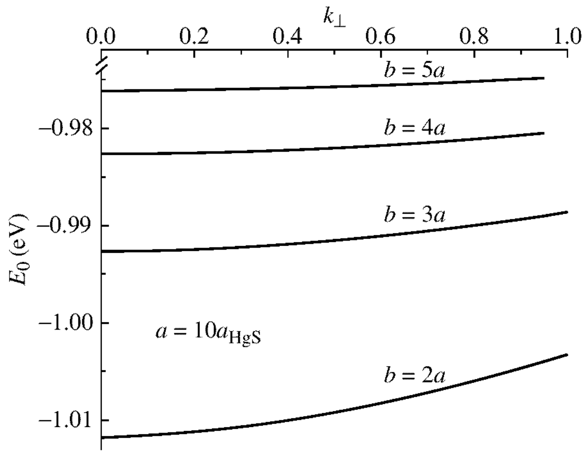

Fig. 2. Electron qround zone dependence on distance between nearest wells, $L = 2\rho_0$.

Figure 2 shows the electron ground band dependence on the distance between the nearest wells (b). It is clear that (b) decreasing shifts the band into the region of lower energies. and increasing its width at the fixed sizes of the well. Physically it means that (b) decreasing is equivalent to the decreasing of barrier height. The electron breely moves in the superlattice i.e. its effective mass of plane movement is decreasing.

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